Electronic and optical properties of a prototype columnar discotic liquid crystal

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Abstract

Structural, electronic, and optical properties calculated for an isolated infinite column of hexakis-hydroxy-triphenylene (HAT0) molecules are presented. This system is intended as a prototype model of columnar discotic liquid crystals since HAT0 is the first member of the discogenic hexakis-n-alkyloxy-triphenylenes (HATn) series; the single-column approximation can be adopted in view of the peculiar nanoseparation of the columns characteristic of these mesophases. Structural optimization of the system has been performed using Car-Parrinello molecular dynamics techniques. Kohn-Sham orbitals, density of states, and electronic energies have been calculated on the optimized structure of the infinite column and implemented in the quantum expression of the transverse dielectric function. The optical absorption spectrum calculated from the dielectric function has been discussed in comparison to a measured absorption spectrum of HAT5 in columnar discotic liquid crystal phase. Optical absorption spectra of short columns of a few HAT0 molecules arranged as in the infinite column have been calculated using the ZINDO method. These spectra are in good agreement with measured absorption spectra of HAT5 and HAT6 in organic solvents, a fact that supports the proposed columnar arrangement of the discotic molecules in these solvents.